```
ANSWER 4 OF 12 CAPLUS COPYRIGHT 2003 ACS on STN
L4
AN
     2001:167995 CAPLUS
DN
     134:207833
     Preparation of tricyclic inhibitors of poly(ADP-ribose) polymerases
TI
     Webber, Stephen Evan; Skalitzky, Donald James; Tikhe, Jayashree Girish;
IN
     Kumpf, Robert Arnold; Marakovits, Joseph Timothy; Eastman, Walter Brian
     Agouron Pharmaceuticals, Inc., USA; Cancer Research Campaign Technology
PA
     Limited
SO
     PCT Int. Appl., 236 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 1
     PATENT NO.
                      KIND
                            DATE
                                           APPLICATION NO.
                            -----
                                           -----
                            20010308
                                           WO 2000-US23882 20000831
     WO 2001016136
                      A2
PΙ
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
             CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
             ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
             LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,
             SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW,
             AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                       A2
                            20020529
                                           EP 2000-961437
                                                           20000831
     EP 1208104
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL
     BR 2000015051
                            20020625
                                           BR 2000-15051
                                                            20000831
                       Α
                                           JP 2001-519702
                            20030408
                                                            20000831
     JP 2003513015
                       T2
     US 6548494
                       B1
                            20030415
                                           US 2000-653184
                                                            20000831
     EE 200200100
                       Α
                            20030616
                                           EE 2002-100
                                                            20000831
                                           NO 2002-421
     NO 2002000421
                       Α
                            20020425
                                                            20020128
                                           BG 2002-106562
                                                            20020329
     BG 106562
                       Α
                            20030331
PRAI US 1999-152142P
                       Р
                            19990831
                            20000831
     WO 2000-US23882
                       W
     MARPAT 134:207833
os
GI
           R6
```

The title compds. [I; X = O, S; Y = N, CR3 (wherein R3 = halo, CN, alkyl, etc.); R1 = H, halo, CN, etc.; R2 = H, alkyl; R4 = H, halo, alkyl; R5-R8 = H, alkyl, alkenyl, aryl, etc.] which are poly(ADP-ribosyl)transferase inhibitors, and are useful in treating cancers and in ameliorating the effects of stroke, head trauma, and neurodegenerative disease, were prepd. E.g., a multi-step synthesis of 1-phenyl-8,9-dihydro-7H-2,7,9a-triaza-benzo[cd]azulen-6-one [I; Y = N; X = O; R1 = Ph; R2, R4-R8 = H] was given. Biol. data for compds. I were presented.

IT 328546-66-3P 328546-75-4P 328546-88-9P

RN 328546-75-4 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 9-amino-7-fluoro-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

RN 328546-88-9 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 9-amino-1,2,3,4-tetrahydro-2-(4-methoxyphenyl)-(9CI) (CA INDEX NAME)

L4 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2003 ACS AN 1978:182987 CAPLUS 88:182987 DN Studies on the imidazo [4,5,1-jk] [1,4] benzodiazepine and TI imidazo[1,5,4-ef][1,5]benzodiazepine series Geneste, P.; Kamenka, J. M.; Vidal, Y.; Fauquet, J. P.; Morel, E.; AU Muller, P.; Warolin, C. Lab. Chim. Org. Phys. Appl., Ec. Natl. Super. Chim., Montpellier, Fr. CS so European Journal of Medicinal Chemistry (1978), 13(1), 53-9 CODEN: EJMCA5; ISSN: 0223-5234 DT Journal French LA GI

AB Of the 7 title compds. (I and II, R = Me or PhCH2; X = O; Y = H, Cl, or NO2) prepd., none showed tranquilizing activity in pentetrazole-induced convulsions or mouse motor activity. The prepn. of I and II from imidazoquinolinones (III) is also described.

IT 66596-64-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction with triethyloxonium fluoroborate)

RN 66596-64-3 CAPLUS

1

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-methyl-(9CI)(CA INDEX NAME)

IT 66596-57-4P 66596-59-6P 66596-60-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and tranquilizing activity of)

RN 66596-57-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-chloro-5,6-dihydro-2-methyl- (9CI) (CA INDEX NAME)

RN 66596-59-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-chloro-5,6-dihydro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 66596-60-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-9-nitro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)

IT 66596-69-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 66596-69-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-methyl-9-nitro-(9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2003 ACS

AN 2002:954525 CAPLUS

DN 138:170205

TI Tricyclic Benzimidazoles as Potent Poly(ADP-ribose) Polymerase-1 Inhibitors

AU Skalitzky, Donald J.; Marakovits, Joseph T.; Maegley, Karen A.; Ekker, Anne; Yu, Xiao-Hong; Hostomsky, Zdenek; Webber, Stephen E.; Eastman, Brian W.; Almassy, Robert; Li, Jianke; Curtin, Nicola J.; Newell, David R.; Calvert, A. Hilary; Griffin, Roger J.; Golding, Bernard T.

CS Pfizer Global R&D, La Jolla/Agouron Pharmaceuticals Inc., San Diego, CA, % 92121, USA

'50 Journal of Medicinal Chemistry (2003), 46(2), 210-213 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

OS CASREACT 138:170205

GI

AB Novel tricyclic benzimidazole carboxamide poly(ADP-ribose) polymerase-1 (PARP-1) inhibitors, e.g., I, have been synthesized. Several compds. were found to be powerful chemopotentiators of temozolomide and topotecan in both A549 and LoVo cell lines. In vitro inhibition of PARP-1 was confirmed by direct measurement of NAD+ depletion and ADP-ribose polymer formation caused by chem. induced DNA damage.

328543-09-5P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (crystal structure; prepn. and MSBAR of tricyclic benzimidazole poly(ADP-ribose)polymerase-l inhibitors via cyclocondensation of aminobenzodiazepine with diethoxymethylbenzaldehyde, hydrolysis, and reductive amination)

RN 328543-09-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(dimethylamino)methyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

Me2N-CH2

### IT 328546-89-0P

RL: BYP (Byproduct); PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study); PREP (Preparation) (prepn., MSBAR, enzymic and cellular activity of tricyclic

benzimidazole poly(ADP-ribose)polymerase-1 inhibitors via cyclocondensation of aminobenzodiazepine with diethoxymethylbenzaldehyde, hydrolysis, and reductive amination)

RN 328546-89-0 CAPLUS

Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

# IT 328543-05-1P 328543-07-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

CN

(Reactant or reagent)

(prepn., MSBAR, enzymic and cellular activity of tricyclic benzimidazole poly(ADP-ribose)polymerase-1 inhibitors via cyclocondensation of aminobenzodiazepine with diethoxymethylbenzaldehyde, hydrolysis, and reductive amination)

RN 328543-05-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(diethoxymethyl)phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328543-07-3 CAPLUS

CN Benzaldehyde, 4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

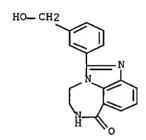
#### IT 328546-77-6P

RL: BYP (Byproduct); PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study); PREP (Preparation)

(prepn., MSBAR, enzymic and cellular activity of tricyclic benzimidazole poly(ADP-ribose)polymerase-1 inhibitors via cyclocondensation of aminobenzodiazepine with dioxolanylbenzaldehyde, hydrolysis, and reductive amination)

RN 328546-77-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)



## IT 328542-63-8P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn., MSBAR, enzymic and cellular activity of tricyclic benzimidazole poly(ADP-ribose)polymerase-1 inhibitors via cyclocondensation of aminobenzodiazepine with dioxolanylbenzaldehyde, hydrolysis, and reductive amination)

RN 328542-63-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-[(dimethylamino)methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

#### IT 328542-61-6P 328543-03-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn., MSBAR, enzymic and cellular activity of tricyclic benzimidazole poly(ADP-ribose)polymerase-1 inhibitors via cyclocondensation of aminobenzodiazepine with dioxolanylbenzaldehyde, hydrolysis, and reductive amination)

RN 328542-61-6 CAPLUS

CN Benzaldehyde, 3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 328543-03-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-(1,3-dioxolan-2-yl)phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

#### IT 328542-20-7P

RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (prepn., MSBAR, enzymic and cellular activity of tricyclic benzimidazole poly(ADP-ribose)polymerase-1 inhibitors via cyclocondensation of aminobenzodiazepine with either acid chlorides or aldehydes)

RN 328542-20-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1-naphthalenyl)- (9CI) (CA INDEX NAME)

# IT 66596-64-3P 328542-04-7P 328542-12-7P 328542-22-9P 328542-30-9P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn., MSBAR, enzymic and cellular activity of tricyclic

benzimidazole poly(ADP-ribose)polymerase-1 inhibitors via cyclocondensation of aminobenzodiazepine with either acid chlorides or aldehydes)

RN 66596-64-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-methyl-(9CI)(CA INDEX NAME)

RN 328542-04-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-phenyl-(9CI) (CA INDEX NAME)

RN 328542-12-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(2-chlorophenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328542-22-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328542-30-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-chlorophenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

#### IT 328542-54-7P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn., MSBAR, enzymic and cellular activity of tricyclic benzimidazole poly(ADP-ribose)polymerase-1 inhibitors via cyclocondensation of aminobenzodiazepine with either acid chlorides or aldehydes and subsequent N-methylation)

RN 328542-54-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-6-methyl-2-(1-naphthalenyl)-(9CI) (CA INDEX NAME)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 2 OF 10 CAPLUS COPYRIGHT 2003 ACS
L4
AN
     2002:428911 CAPLUS
DN
     137:6205
     Preparation of benzazepinones, isoquinolinones and related compounds as
ΤI
     inhibitors of poly(ADP-ribose) polymerase (PARP) for the prevention
     and/or treatment of tissue damage from cell trauma or cell death due to
     necrosis or apoptosis.
     Ferraris, Dana V.; Li, Jia-He; Kalish, Vincent J.; Zhang, Jie
IN
     Guilford Pharmaceuticals Inc., USA
PA
     PCT Int. Appl., 152 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
LΑ
FAN.CNT 1
     PATENT NO.
                      KIND
                                            APPLICATION NO.
                                                             DATE
                                            WO 2001-US44815
                                                             20011130
                       A2
                            20020606
PΙ
     WO 2002044183
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
             US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                           AU 2002-36521
     AU 2002036521
                            20020611
                                                             20011130
                       A5
                                            US 2001-996776
                                                             20011130
     US 2003022883
                       A1
                            20030130
PRAI US 2000-250132P
                       P
                            20001201
     US 2001-310274P
                       P
                            20010809
     WO 2001-US44815
                       W
                            20011130
     MARPAT 137:6205
OS
GI
                                             R12
                                             R11
```

AB This invention discloses the prepn. of title compds. I and II, their pharmaceutically acceptable salts, and related compds. as inhibitors of poly(ADP-ribose) polymerase (PARP) [wherein: A = N, C, CH2, CH; B = C,

NH, S, SO, SO2; X = C, CH, N; Y = C, N; Z = C, CH2, N, CO; provided that at least one of X, Y, or Z is N; R1, R2, R3, R5 when present are optionally or independently = H, OH, :O, (un) substituted alkyl, alkenyl, alkoxy, carboxy, cycloalkyl, heterocycloalkyl, aryl,

heteroaryl,

halogen, amine, COR8 (R8 = H, OH, (un) substituted alkyl, alkenyl, alkynyl,

alkoxy, carboxy, cycloalkyl, heterocycloalkyl, aryl, heteroaryl), OR6,
 NR6R7 (R6, R7 independently = H, (un)substituted alkyl, alkenyl,
alkynyl,

cycloalkyl, heterocycloalkyl, aryl, heteroaryl); R1, R2, R3, R5 optionally

form ring through a straight or branched C1-4alkyl which may addnl. contain 1-2 double or triple bonds; R4 = 1-3 of H, halo, or alkyl; with proviso that when A, X, or Z = C, then R1, R2, R3 when present may also independently = halogen, CN, O; R9, R10, R11, R12 optionally or independently = H, halogen, amino, OH, halo-amine, O-alkyl, O-aryl, (un)substituted alkyl, alkenyl, alkynyl, alkoxy, carboxy, cycloalkyl, heterocycloalkyl, aryl, heteroaryl, COR8; R13 = 1-3 of H, halogen, alkoxy,

alkyl]. For example, cyclocondensation of formylindazole III (prepd. from

Me indole-4-carboxylate and NaNO2/AcOH), with hydrazine provided claimed benzoazulenone IV as a white solid. Benzoazulenone IV inhibited human recombinant PARP at an IC50 of 0.018 .mu.M. PARP IC50 inhibition studies

for an addnl. 156 examples are provided, ranging in values from 0.01 to  $20\,$ 

.mu.M. Biol. data are provided for the in vivo treatment of focal cerebral ischemia and gout via PARP inhibition with selected compds. II. The present invention is believed to protect cells, tissue and organs against the ill-effects of reactive free radicals and nitric oxide through

inhibition of PARP activity.

IT 433726-34-2P 433726-44-4P 433726-45-5P 433726-49-9P 433726-62-6P 433727-33-4P 433727-80-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; prepn. of benzazepinones, isoquinolinones and related

compds. as inhibitors of poly(ADP-ribose) polymerase (PARP))

RN 433726-34-2 CAPLUS

CN Benzoic acid, 3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN

CN Benzoic acid, 4-[2-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)ethyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 433726-45-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[2-[4-(hydroxymethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

RN 433726-49-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(chloromethyl)-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433726-62-6 CAPLUS

CN Benzoic acid, 4-[2-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-

RN 433727-33-4 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(2,5-diazabicyclo[2.2.1]hept-2-ylmethyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

IT

```
328542-16-1P 328542-18-3P 328542-20-7P
328542-24-1P 328542-40-1P 328542-42-3P
328542-43-4P 328542-48-9P 328542-52-5P
328543-09-5P 328543-52-8P 328543-80-2P
328543-82-4P 328544-31-6P 328545-93-3P
328545-96-6P 328546-21-0P 328546-89-0P
328547-10-0P 433726-06-8P 433726-07-9P
433726-08-0P 433726-09-1P 433726-10-4P
433726-11-5P 433726-12-6P 433726-13-7P
433726-14-8P 433726-15-9P 433726-16-0P
433726-17-1P 433726-18-2P 433726-19-3P
433726-20-6P 433726-21-7P 433726-22-8P
433726-23-9P 433726-24-0P 433726-25-1P
433726-26-2P 433726-27-3P 433726-28-4P
433726-29-5P 433726-30-8P 433726-31-9P
433726-32-0P 433726-33-1P 433726-35-3P
433726-36-4P 433726-37-5P 433726-38-6P
433726-39-7P 433726-40-0P 433726-41-1P
433726-42-2P 433726-43-3P 433726-46-6P
433726-47-7P 433726-48-8P 433726-50-2P
433726-51-3P 433726-52-4P 433726-53-5P
433726-54-6P 433726-55-7P 433726-56-8P
433726-57-9P 433726-58-0P 433726-59-1P
433726-60-4P 433726-61-5P 433726-63-7P
433726-95-5P 433726-96-6P 433726-97-7P
433726-98-8P 433727-00-5P 433727-01-6P
433727-02-7P 433727-03-8P 433727-04-9P
433727-05-0P 433727-06-1P 433727-07-2P
433727-08-3P 433727-09-4P 433727-10-7P
433727-11-8P 433727-12-9P 433727-13-0P
433727-14-1P 433727-15-2P 433727-16-3P
433727-17-4P 433727-18-5P 433727-19-6P
433727-20-9P 433727-21-0P 433727-22-1P
433727-23-2P 433727-24-3P 433727-25-4P
433727-26-5P 433727-27-6P 433727-28-7P
433727-29-8P 433727-30-1P 433727-31-2P
433727-32-3P 433727-34-5P 433727-35-6P
433727-36-7P 433727-37-8P 433727-38-9P
433727-39-0P 433727-40-3P 433727-41-4P
433727-42-5P 433727-43-6P 433727-44-7P
433727-45-8P 433727-46-9P 433727-47-0P
433727-48-1P 433727-49-2P 433727-50-5P
433727-51-6P 433727-52-7P 433727-53-8P
433727-54-9P 433727-55-0P 433727-56-1P
433727-57-2P 433727-58-3P 433727-59-4P
433727-60-7P 433727-61-8P 433727-62-9P
433727-63-0P 433727-64-1P 433727-65-2P
433727-66-3P 433727-67-4P 433727-68-5P
433727-69-6P 433727-70-9P 433727-71-0P
433727-72-1P 433727-73-2P 433727-74-3P
433727-75-4P 433727-76-5P 433727-77-6P
433727-78-7P 433727-79-8P 433727-81-2P
433727-82-3P 433727-83-4P 433727-84-5P
433727-85-6P 433727-86-7P 433727-87-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
```

RN 328542-04-7 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-phenyl(9CI)
(CA INDEX NAME)

RN 328542-06-9 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-fluorophenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328542-16-1 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(3-pyridinyl)(9CI) (CA INDEX NAME)

RN 328542-18-3 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-thienyl)(9CI) (CA INDEX NAME)

RN 328542-20-7 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 328542-24-1 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 328542-40-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-phenylethyl)- (9CI) (CA INDEX NAME)

RN 328542-42-3 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(2-furanyl)-5,6-dihydro(9CI) (CA INDEX NAME)

RN 328542-48-9 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-cyclohexyl-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328542-52-5 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepine-2,7(1H,4H)-dione, 5,6-dihydro-(9CI)
(CA INDEX NAME)

NH

RN 328543-09-5 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4[(dimethylamino)methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

Me2N-CH2

RN 328543-52-8 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1H-imidazol2-yl)- (9CI) (CA INDEX NAME)

RN 328543-80-2 CAPLUS CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1H-pyrrol-2-yl)- (9CI) (CA INDEX NAME)

RN 328543-82-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[5-(4-chlorophenyl)-2-furanyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328544-31-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[3-(dimethylamino)propoxy]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328545-93-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(3,4-dihydro-2(1H)-isoquinolinyl)methyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328545-96-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[methyl(phenylmethyl)amino]methyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328546-21-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-pyrrolidinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328547-10-0 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(chloromethyl)phenyl]5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433726-06-8 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(3-methylphenyl)- (9CI) (CA INDEX NAME)

RN 433726-07-9 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(4-methylphenyl)- (9CI) (CA INDEX NAME)

RN 433726-08-0 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-bromophenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433726-09-1 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(3,5-difluorophenyl)5,6dihydro- (9CI) (CA INDEX NAME)

RN 433726-10-4 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(2,4-dihydroxyphenyl)5,6dihydro- (9CI) (CA INDEX NAME)

RN 433726-11-5 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 433726-12-6 CAPLUS CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1-methyl-1H-indol-3-yl)- (9CI) (CA INDEX NAME)

RN 433726-13-7 CAPLUS
CN Benzoic acid, 4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 433726-14-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(3,4,5-trihydroxyphenyl)- (9CI) (CA INDEX NAME)

RN 433726-15-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(2-fluorophenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433726-16-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-quinolinyl)- (9CI) (CA INDEX NAME)

RN 433726-17-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[2-(4-methoxyphenyl)-1-methylethyl]- (9CI) (CA INDEX NAME)

RN 433726-18-2 CAPLUS

CN Cyclopropanecarboxylic acid, 2-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)-, ethyl ester, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 433726-19-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(methoxymethyl)- (9CI) (CA INDEX NAME)

RN 433726-20-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[2-(4-methoxyphenyl)ethenyl]- (9CI) (CA INDEX NAME)

RN 433726-21-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[(phenylmethoxy)methyl]- (9CI) (CA INDEX NAME)

RN 433726-22-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(phenylethynyl)- (9CI) (CA INDEX NAME)

RN 433726-23-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(5-nitro-2-furanyl)- (9CI) (CA INDEX NAME)

RN 433726-24-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[5-[(acetyloxy)methyl]-

2furanyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433726-25-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-phenylethenyl)- (9CI) (CA INDEX NAME)

RN 433726-26-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[[methyl(phenylmethyl)amino]methyl]- (9CI) (CA INDEX NAME)

RN 433726-27-3 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1-pyrrolidinylmethyl)- (9CI) (CA INDEX NAME)

RN 433726-28-4 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(2,2-diphenylethenyl)5,6dihydro- (9CI) (CA INDEX NAME)

RN 433726-29-5 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(3-bromophenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433726-30-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[5-(3-chlorophenyl)-2-furanyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433726-31-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[5-(2-chlorophenyl)-2-furanyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433726-32-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(5-bromo-2-thienyl)-

5,6dihydro- (9CI) (CA INDEX NAME)

RN 433726-33-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepine-2-propanoic acid, 4,5,6,7-tetrahydro-7-oxo- (9CI) (CA INDEX NAME)

RN 433726-35-3 CAPLUS

CN Piperazine, 1-methyl-4-[3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)benzoyl]- (9CI) (CA INDEX NAME)

RN 433726-36-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[[5-(phenylmethyl)-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]- (9CI) (CA INDEX

NAME)

RN 433726-37-5 CAPLUS

CN Benzamide, N-[3-(dimethylamino)propyl]-N-methyl-3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 433726-38-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[(dimethylamino)methyl]-

5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433726-39-7 CAPLUS

CN L-Tyrosine, N-[1-oxo-3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)propyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433726-40-0 CAPLUS

CN Glycine, N-[1-oxo-3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)propyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 433726-41-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[5-[2-chloro-5-(trifluoromethyl)phenyl]-2-furanyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433726-42-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[5-(3-fluorophenyl)-2,5-

diazabicyclo[2.2.1]hept-2-yl]methyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433726-43-3 CAPLUS

CN L-Phenylalanine, N-[1-oxo-3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)propyl}-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433726-46-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepine-2-propanamide, 4,5,6,7-tetrahydro-

N[2-(4-hydroxyphenyl)ethyl]-7-oxo- (9CI) (CA INDEX NAME)

PAGE 1-A

RN 433726-47-7 CAPLUS

1H-

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1-methyl-

pyrrol-2-yl)- (9CI) (CA INDEX NAME)

RN 433726-48-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[2-[4-(1-pyrrolidinylmethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

RN 433726-50-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepine-2-propanamide, 4,5,6,7-tetrahydro-

N-

[2-(3-methoxyphenyl)ethyl]-7-oxo- (9CI) (CA INDEX NAME)

PAGE 1-A

RN 433726-51-3 CAPLUS CN Imidazo[4,5,1-jk][1,

Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1-methyl-

1H- imidazol-2-yl)- (9CI) (CA INDEX NAME)

7-

RN 433726-52-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepine-2-propanamide, 4,5,6,7-tetrahydro-

oxo-N-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

RN 433726-53-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[5-(3-nitrophenyl)-2-furanyl]- (9CI) (CA INDEX NAME)

RN 433726-54-6 CAPLUS

CN Carbamic acid, [(1R)-2-phenyl-1-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433726-55-7 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(1-amino-2-phenylethyl)5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433726-56-8 CAPLUS
CN Benzoic acid, 4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)-, methyl ester (9CI) (CA INDEX NAME)

RN 433726-57-9 CAPLUS
CN 1H-Pyrrole-2-carboxaldehyde, 1-methyl-5-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 433726-58-0 CAPLUS

CN 1H-Pyrrole-3-carboxaldehyde, 1-methyl-5-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 433726-59-1 CAPLUS

CN Piperazine, 1-methyl-4-[[5-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)-2-furanyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 433726-60-4 CAPLUS

CN 2-Furancarboxylic acid, 5-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 433726-61-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4,5-dimethyl-2-furanyl)-

5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433726-63-7 CAPLUS

CN Glycine, N-methyl-N-[(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 433726-95-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433726-96-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(3-chlorophenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433726-97-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(3,5-dihydroxyphenyl)-

5,6-

dihydro- (9CI) (CA INDEX NAME)

RN 433726-98-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(1-amino-2-

phenylethyl)-

5,6-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 433727-00-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(5-nitro-2-

thienyl) - (9CI) (CA INDEX NAME)

RN 433727-01-6 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(5-amino-2-furanyl)5,6dihydro- (9CI) (CA INDEX NAME)

RN 433727-02-7 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1-piperidinylmethyl)- (9CI) (CA INDEX NAME)

RN 433727-03-8 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1H-imidazol1-ylmethyl)- (9CI) (CA INDEX NAME)

RN 433727-04-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[(3,4-dihydro-1(2H)-quinolinyl)methyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433727-05-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[(methylphenylamino)methyl]- (9CI) (CA INDEX NAME)

RN 433727-06-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[(4-methyl- $\frac{1}{2}$ )

1 piperazinyl)methyl]- (9CI) (CA INDEX NAME)

RN 433727-08-3 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2[(cyclohexylmethylamino)methyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433727-09-4 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[(4-phenyl-1-piperazinyl)methyl]- (9CI) (CA INDEX NAME)

RN 433727-10-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[(dibutylamino)methyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433727-11-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[[3-(dimethylamino)propyl]methylamino]methyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433727-12-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[(4-oxo-1-piperidinyl)methyl]- (9CI) (CA INDEX NAME)

RN 433727-13-0 CAPLUS

CN 3-Piperidinecarboxylic acid, 4-oxo-1-[(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 433727-14-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[[2-(hydroxymethyl)-1-piperidinyl]methyl]- (9CI) (CA INDEX NAME)

RN 433727-15-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[(hexahydro-1H-azepin-1-

yl)methyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433727-16-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(4-morpholinylmethyl)- (9CI) (CA INDEX NAME)

RN 433727-17-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[[4-(phenylmethyl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)

RN 433727-18-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[(hexahydroazocin-1(2H)-

yl)methyl]~5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433727-19-6 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2[(dipentylamino)methyl]5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433727-20-9 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[(dihexylamino)methyl]5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433727-21-0 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-{[bis(1-methylethyl)amino]methyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433727-22-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[(diethylamino)methyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433727-23-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[[(4-methoxyphenyl)methylamino]methyl]- (9CI) (CA INDEX NAME)

RN 433727-24-3 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2[(dipropylamino)methyl]5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433727-25-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[bis(phenylmethyl)amino]methyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433727-26-5 CAPLUS

CN l-Piperazinecarboxylic acid, 4-[(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 433727-27-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[4-(1,3-benzodioxol-5-ylmethyl)-1-piperazinyl]methyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 433727-28-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[[2-(dimethylamino)ethyl](phenylmethyl)amino]methyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433727-29-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[[(2-phenylethyl)(phenylmethyl)amino]methyl]- (9CI) (CA INDEX NAME)

RN 433727-30-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[(3,4-dihydro-2(1H)-isoquinolinyl)methyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433727-31-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)methyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433727-32-3 CAPLUS

CN L-Proline, 1-[(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-

jk][1,4]benzodiazepin-

2-yl)methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433727-34-5 CAPLUS

CN Benzamide, N-[2-(4-morpholinyl)ethyl]-3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 433727-35-6 CAPLUS

CN Benzamide, N-[2-(1-pyrrolidinyl)ethyl]-3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 433727-36-7 CAPLUS

CN Benzamide, N-[2-(1-piperidinyl)ethyl]-3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 433727-37-8 CAPLUS

CN Piperazine, 1-(phenylmethyl)-4-[3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-

jk][1,4]benzodiazepin-2-yl)benzoyl]- (9CI) (CA INDEX NAME)

RN 433727-38-9 CAPLUS

CN Piperazine, 1-(1,3-benzodioxol-5-ylmethyl)-4-[3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)benzoyl]- (9CI) (CA INDEX NAME)

RN 433727-39-0 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-

jk][1,4]benzodiazepin-2-yl)benzoyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 433727-40-3 CAPLUS

CN Benzamide, N-[2-(1-methyl-2-pyrrolidinyl)ethyl]-3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \\ \text{N} \\ \text{CH}_2\text{-CH}_2\text{-NH} \\ \\ \text{N} \\$$

RN 433727-41-4 CAPLUS

CN Benzamide, N-[2-(diethylamino)ethyl]-3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 433727-42-5 CAPLUS

CN Benzamide, N-[2-(dimethylamino)ethyl]-3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 433727-43-6 CAPLUS

CN Benzamide, N-[3-(diethylamino)propyl]-3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 433727-44-7 CAPLUS

CN 2,5-Diazabicyclo[2.2.1]heptane, 2-(phenylmethyl)-5-[3-(4,5,6,7-tetrahydro-

7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)benzoyl]- (9CI) (CA INDEX NAME)

RN 433727-45-8 CAPLUS

CN 3-Piperidineacetic acid, 4-oxo-1-[3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-

jk][1,4]benzodiazepin-2-yl)benzoyl]- (9CI) (CA INDEX NAME)

RN 433727-46-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[5-[(2,5-dimethylphenyl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433727-47-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[[5-[(3-methoxyphenyl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]- (9CI)

(CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & & \text{CH}_2 & & \text{N} \\ \hline \\ \text{CH}_2 & & & \text{N} \\ \hline \\ \text{O} & & & \\ \end{array}$$

RN 433727-48-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[[5-[(4-methoxyphenyl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]- (9CI)

(CA INDEX NAME)

RN 433727-49-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[5-[[4-(acetyloxy)phenyl]methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433727-50-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[5-[(3,4-dimethylphenyl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]-5,6-

dihydro- (9CI) (CA INDEX NAME)

RN 433727-51-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[5-[(3,4-dichlorophenyl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433727-52-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[5-[[4-(1,1-dimethylethyl)phenyl]methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]-5,6-

dihydro- (9CI) (CA INDEX NAME)

RN 433727-53-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[[5-[(4-methylphenyl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]- (9CI)

(CA INDEX NAME)

RN 433727-54-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[5-[(4-fluorophenyl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]-5,6-dihydro-

(9CI) (CA INDEX NAME)

RN 433727-55-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[5-[(3-chlorophenyl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]-5,6-dihydro-

(9CI) (CA INDEX NAME)

$$CH_2$$
  $N$   $CH_2$   $N$ 

RN 433727-56-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[5-[(2-fluorophenyl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]-5,6-dihydro-

(9CI) (CA INDEX NAME)

RN 433727-57-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[[5-[(3-

Me 
$$CH_2$$
  $N$   $CH_2$   $N$ 

RN 433727-58-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[[5-[(2-methylphenyl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]- (9CI)

(CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \\ & \text{CH}_2 & \\ & \text{N} & \\ & \text{CH}_2 & \\ & \text{N} & \\ & \text{O} & \\ & \text{O} & \\ & \text{N} & \\ & \text{O} & \\ & \text{O}$$

RN 433727-59-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[5-{(3-fluorophenyl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]-5,6-dihydro-

(9CI) (CA INDEX NAME)

RN 433727-60-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[5-[(2-chlorophenyl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]-5,6-dihydro-

(9CI) (CA INDEX NAME)

RN 433727-61-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[[5-[[4-[(1E)-

2-phenylethenyl]phenyl]methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 433727-62-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[[5-[[4-(phenylmethoxy)phenyl]methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]-(9CI) (CA INDEX NAME)

RN 433727-63-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[5-[(6-chloro-1,3-benzodioxol-5-yl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
CH_2 & N & CH_2 \\
\hline
C1 & N & CH_2 \\
\hline
N & N & C$$

RN 433727-64-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[[5-[(4-k)]]]

 ${\tt chlorophenyl)\,methyl]-2,5-diazabicyclo\{2.2.1]\,hept-2-yl]\,methyl]-5,6-dihydro-$ 

(9CI) (CA INDEX NAME)

RN 433727-65-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[2-[4-[(dimethylamino)methyl]phenyl]ethyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433727-66-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[2-[4-[[2-(hydroxymethyl)-1-piperidinyl]methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

1/

RN 433727-67-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[2-[4-[(4-methyl-1-piperazinyl)methyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



RN 433727-68-5 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[2-[4-[(3,4-dihydro-2(1H)-isoquinolinyl)methyl]phenyl]ethyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433727-70-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[2-[4-(1-pyrrolidinylmethyl)phenyl]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

RN 433727-71-0 CAPLUS

CN 2,5-Diazabicyclo[2.2.1]heptane, 2-(phenylmethyl)-5-[4-[2-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)ethyl]benzoyl]-(9CI) (CA INDEX NAME)

RN 433727-72-1 CAPLUS

CN Piperazine, 1-(phenylmethyl)-4-[4-[2-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)ethyl]benzoyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

CN Benzamide, N-[2-(1-pyrrolidinyl)ethyl]-4-[2-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 433727-74-3 CAPLUS
CN Benzamide, N-[2-(1-piperidinyl)ethyl]-4-[2-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)ethyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 433727-75-4 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[4-[2-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)ethyl]benzoyl]-, methyl ester

(9CI) (CA INDEX NAME)

PAGE 2-A

RN 433727-76-5 CAPLUS
CN Benzamide, N-[2-(diethylamino)ethyl]-4-[2-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)ethyl]- (9CI) (CA INDEX

NAME)

RN 433727-77-6 CAPLUS

CN Piperazine, 1-methyl-4-[4-[2-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)ethyl]benzoyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 433727-78-7 CAPLUS

CN 3-Piperidinecarboxylic acid, 4-oxo-1-[4-[2-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)ethyl]benzoyl]-, methyl ester

(9CI) (CA INDEX NAME)

RN 433727-79-8 CAPLUS
CN Benzamide, N-[2-(dimethylamino)ethyl]-N-methyl-4-[2-(4,5,6,7-tetrahydro-7oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)ethyl]- (9CI) (CA INDEX
NAME)

RN 433727-81-2 CAPLUS
CN Glycine, N-[4-[2-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)ethyl]benzoyl]- (9CI) (CA INDEX NAME)

RN 433727-82-3 CAPLUS
CN 4-Piperidinecarboxylic acid, 1-[[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]methyl]-, methyl ester (9CI) (CA INDEX
NAME)

PAGE 1-A

RN 433727-83-4 CAPLUS
CN Glycine, N-methyl-N-[[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 433727-84-5 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[[2-(dimethylamino)ethyl]methylamino]methyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 433727-85-6 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(4-methyl1-piperazinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 433727-86-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[2-(hydroxymethyl)-1-piperidinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 433727-87-8 CAPLUS

CN Glycine, N-methyl-N-[[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]methyl]-, 1,1-dimethylethyl ester (9CI)

(CA INDEX NAME)

## IT 433728-62-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(intermediate; prepn. of benzazepinones, isoquinolinones and related compds. as inhibitors of poly(ADP-ribose) polymerase (PARP))

RN 433728-62-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[2-[4-(chloromethyl)phenyl]ethyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

```
ANSWER 3 OF 10 CAPLUS COPYRIGHT 2003 ACS
L4
     2002:408675 CAPLUS
AN
DN
     136:401791
     Benzimidazole derivatives, specifically imidazo[4,5,1-
TI
     j,k][1,4]benzodiazepin-7(4H)-one derivatives, and the preparation and
     therapeutic use thereof as inhibitors of poly(ADP-ribose)polymerase
     (PARP).
     Barth, Francis; Bichon, Daniel; Bolkenius, Frank; Van Dorsselaer,
IN
     Viviane
     Sanofi-Synthelabo, Fr.
PA
     PCT Int. Appl., 48 pp.
SO
     CODEN: PIXXD2
DТ
     Patent
LΑ
     French
FAN.CNT 1
                                            APPLICATION NO.
                                                             DATE
     PATENT NO.
                      KIND
                             DATE
                             20020530
                                            WO 2001-FR3667
ΡI
     WO 2002042306
                       A1
                                                              20011121
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA,
             UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ,
TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                            FR 2000-15141
                                                             20001123
     FR 2816941
                       A1
                             20020524
     FR 2816941
                       B1
                             20030131
     FR 2816942
                             20020524
                                            FR 2001-6157
                                                              20010510
                       A1
     FR 2816942
                             20030509
                       В1
     AU 2002022003
                       A5
                             20020603
                                            AU 2002-22003
                                                             20011121
PRAI FR 2000-15141
                       Α
                             20001123
     FR 2001-6157
                             20010510
                       Α
     WO 2001-FR3667
                       W
                            20011121
OS
     MARPAT 136:401791
GI
```

The invention concerns fused benzimidazole derivs. I, including their enantiomers, diastereomers, mixts., racemates, free bases, and pharmaceutically acceptable acid addn. salts [wherein: R1 = H, C1-4 alkyl or alkoxy, halo, NO2; R2, R2', R9, R9' = H, C1-4 alkyl; X = N or C; m = 1 or 2; when X = N, then R3 = H, C1-C4 alkyl, or is absent, and R4 = in particular H, C1-C6 alkyl, C3-C7 cycloalkyl, (un)substituted 4-piperidyl, (CH2)pNR5R6, (CH2)pCONR5R6, CO(CH2)pNR5R6, (un)substituted (CH2)pPh, (CH2)p-morpholinyl, (CH2)p-pyrrolidinyl, (CH2)p-tetrahydroisoquinoline, (CH2)p-heteoraryl, heteroarylcarbonyl,

phenylcarbonyl, C1-C6

alkylcarbonyl, (CH2)pCOOR', or SO2Ph; when X = C, then R3 = H, NR5R6,

NHCOR7, CONHR5, COR7, NHCONH2, OH, or CH2OH, and R4 = in particular H, (un) substituted (CH2)pPh, (CH2)p-heteroaryl, or (CH2)tNR7R8; p = 0-4; t

O or 1; R5, R6 = H, C1-4 alkyl; R7, R8 = C1-4 alkyl or alkoxy, or may together form an (un)substituted satd. ring of 5-7 members, optionally contg. an addnl. N atom]. I can be used for prepg. medicines for treating

or preventing a wide variety of disorders wherein the PARP enzyme is involved. A table of 38 compds. I and salts is given. For instance, 4H-imidazo[4,5,1-ij]quinolin-2,6(1H,5H)-dione underwent chlorination of the 2-oxo group with POCl3 and NH4Cl, and then ring-expansion at the 6-

group using NaN3 and H2SO4. The resultant intermediate, 2-chloro-5,6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, reacted

with 1-phenylpiperazine in the presence of 2,6-lutidine and CsF, in triethylene glycol monomethyl ether at 140.degree., to give title compd. II in 53% yield. The most active compds. I inhibited human recombinant PARP-1 and/or PARP-2 in vitro with IC50 values of 5-500 nM.

IT 429689-48-5P, 2-[4-[(tert-Butyloxy)carbonyl]piperazin-1-yl]-5methyl-5,6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; prepn. of benzimidazole derivs. as PARP inhibitors) 429689-48-5 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-(4,5,6,7-tetrahydro-5-methyl-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

oxo

RN

1T 429689-42-9P, 2-(4-Phenylpiperazin-1-yl)-5,6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-43-0P,
2-[4-(4-Pyridyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-44-1P,
2-[4-(1-Piperidyl)piperidin-1-yl]-5,6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-45-2P,
2-[4-(5-Methyl-1H-imidazol-4-yl)piperidin-1-yl]-5,6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-46-3P,
2-(4-Phenylpiperazin-1-yl)-5-methyl-5,6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-47-4P,

```
2-(4-Methylpiperazin-1-yl)-5,6-dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-
7(4H)-one 429689-49-6P, 2-[4-(2-Pyridyl)piperazin-1-yl]-5,6-
dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-50-9P
, 2-(Piperazin-1-yl)-5-methyl-5,6-dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one dihydrochloride 429689-51-0P,
2-(4-Acetylpiperazin-1-yl)-5-methyl-5,6-dihydroimidazo[4,5,1-
jk] [1,4]benzodiazepin-7(4H)-one 429689-52-1P,
2-[4-(4-Nitrophenyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-
jk] [1, 4] benzodiazepin-7(4H)-one 429689-53-2P,
2-[4-(4-Fluorophenyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one 429689-54-3P,
2-[4-(2-Chlorophenyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one 429689-55-4P,
2-(4-Methylhomopiperazin-1-yl)-5,6-dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one 429689-56-5P,
2-[4-[(tert-Butyloxy)carbonyl]piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one 429689-57-6P,
2-(Piperazin-1-y1)-5,6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-
one dihydrochloride 429689-58-7P, 2-[4-Phenyl-4-[[(tert-
butyloxy) carbonyl] amino] piperidin-1-yl]-5, 6-dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one 429689-59-8P,
2-[4-(2-Morpholinoethyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one 429689-60-1P,
2-[4-(1-Methylpiperidin-4-yl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-
jk] [1,4]benzodiazepin-7(4H)-one 429689-61-2P,
2-(4-Phenyl-4-aminopiperidin-1-yl)-5,6-dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one dihydrochloride 429689-62-3P,
2-[4-[[(Diethylamino)carbonyl]methyl]piperazin-1-yl]-5,6-
dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-63-4P
, 2-[4-(3-Pyrrolidinopropyl)homopiperazin-1-yl]-5,6-
dihvdroimidazo[4,5,1-
jk] [1,4]benzodiazepin-7(4H)-one 429689-64-5P,
2-[4-[3-(Dimethylamino)propyl]piperazin-1-yl]-5-methyl-5,6-
dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-65-6P
, 2-[4-[(4-Pyridinyl)methyl]piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one 429689-66-7P,
2-[4-[4-(Trifluoromethyl)phenyl]piperazin-1-yl]-5,6-
dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one 429689-67-8P,
2-[4-(3-Phenylpropyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one 429689-68-9P,
2-[4-(2-Fluorophenyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one 429689-69-0P,
2-[4-[(3,5-Dimethyl-1-phenylpyrazol-4-yl)methyl]piperazin-1-yl]-5,6-
dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-70-3P
, 2-[4-[5-(4-Fluorophenyl)pyrazol-3-yl]piperidin-1-yl]-5,6-
dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-71-4P
, 2-(4-Cyclohexylpiperazin-1-yl)-5,6-dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one 429689-72-5P,
2-[4-[3-(1,2,3,4-Tetrahydroisoquinolin-2-yl)propyl]piperazin-1-yl]-5,6-
dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-73-6P
, 2-[4-(4-Fluorophenyl)piperazin-1-yl]-10-methyl-5,6-
dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one 429689-74-7P,
2-(4-Cyclohexylpiperazin-1-yl)-10-methyl-5,6-dihydroimidazo[4,5,1-
jk][1,4]benzodiazepin-7(4H)-one 429689-75-8P,
```

2-[4-(4-Fluorophenyl)piperazin-1-yl]-8-methyl-5,6-dihydroimidazo[4,5,1jk] [1,4]benzodiazepin-7(4H)-one 429689-76-9P, 2-[4-(4-Fluorophenyl)piperazin-1-yl]-9-methyl-5,6-dihydroimidazo[4,5,1jk] [1,4]benzodiazepin-7(4H)-one 429689-77-0P, 2-[4-(4-Fluorophenyl)piperazin-1-yl]-4-propyl-5,6-dihydroimidazo[4,5,1jk][1,4]benzodiazepin-7(4H)-one 429689-78-1P, 2-[4-[(Dimethylamino)acetyl]piperazin-1-yl]-5,6-dihydroimidazo[4,5,1jk][1,4]benzodiazepin-7(4H)-one 429689-79-2P, 2-[4-(4-Hydroxyphenyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1jk][1,4]benzodiazepin-7(4H)-one RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (drug candidate; prepn. of benzimidazole derivs. as PARP inhibitors) RN 429689-42-9 CAPLUS CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(4-phenyl-1-piperazinyl) - (9CI) (CA INDEX NAME)

RN 429689-43-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-pyridinyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 429689-44-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[1,4'-bipiperidin]-1'-y1-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 429689-46-3 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-methyl-2-(4phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

RN 429689-47-4 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(4-methyl1piperazinyl)- (9CI) (CA INDEX NAME)

RN 429689-49-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(2-pyridinyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 429689-50-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-methyl-2-

(1piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)

## ●2 HCl

RN 429689-51-0 CAPLUS

CN Piperazine, 1-acetyl-4-(4,5,6,7-tetrahydro-5-methyl-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 429689-52-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-nitrophenyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 429689-53-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(4-fluorophenyl)-1-piperazinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 429689-54-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(2-chlorophenyl)-1-piperazinyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 429689-55-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 429689-56-5 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 429689-57-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

RN 429689-58-7 CAPLUS

CN Carbamic acid, [4-phenyl-1-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)-4-piperidinyl]-, 1,1-dimethylethyl ester (9CI)

(CA INDEX NAME)

RN 429689-59-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[2-(4-morpholinyl)ethyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 429689-60-1 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-methyl-4-piperidinyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 429689-61-2 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-amino-4-phenyl-1-piperidinyl)-5,6-dihydro-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

RN 429689-62-3 CAPLUS
CN 1-Piperazineacetamide, N,N-diethyl-4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 429689-63-4 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[hexahydro-4-[3-(1-pyrrolidinyl)propyl]-1H-1,4-diazepin-1-yl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 429689-64-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[3-(dimethylamino)propyl]-1-piperazinyl]-5,6-dihydro-5-methyl- (9CI) (CA INDEX NAME)

RN 429689-65-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-pyridinylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 429689-66-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[4-(trifluoromethyl)phenyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 429689-67-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(3-phenylpropyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 429689-68-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(2-fluorophenyl)-1-piperazinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 429689-69-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(3,5-dimethyl-1-phenyl-1H-pyrazol-4-yl)methyl]-1-piperazinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 429689-70-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[5-(4-fluorophenyl)-

1Hpyrazol-3-yl]-1-piperidinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

1/2

RN 429689-71-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-cyclohexyl-1-piperazinyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 429689-72-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[3-(3,4-dihydro-2(1H)-

isoquinolinyl)propyl]-1-piperazinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 429689-73-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(4-fluorophenyl)-1-piperazinyl]-5,6-dihydro-10-methyl- (9CI) (CA INDEX NAME)

RN 429689-74-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-cyclohexyl-1-piperazinyl)-5,6-dihydro-10-methyl- (9CI) (CA INDEX NAME)

RN 429689-75-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(4-fluorophenyl)-1-piperazinyl]-5,6-dihydro-8-methyl- (9CI) (CA INDEX NAME)

RN 429689-76-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(4-fluorophenyl)-1-piperazinyl]-5,6-dihydro-9-methyl- (9CI) (CA INDEX NAME)

RN 429689-77-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(4-fluorophenyl)-1-piperazinyl]-5,6-dihydro-4-propyl- (9CI) (CA INDEX NAME)

RN 429689-78-1 CAPLUS

CN Piperazine, 1-[(dimethylamino)acetyl]-4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 429689-79-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-hydroxyphenyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

429689-80-5P, 2-Chloro-5, 6-dihydroimidazo[4,5,1-IT jk][1,4]benzodiazepin-7(4H)-one 429689-81-6P, 2-Chloro-5-methyl-5, 6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)one 429689-82-7P, 2-Chloro-10-methyl-5,6-dihydroimidazo[4,5,1jk][1,4]benzodiazepin-7(4H)-one RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; prepn. of benzimidazole derivs. as PARP inhibitors) RN 429689-80-5 CAPLUS Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-chloro-5,6-dihydro-CN (9CI) (CA INDEX NAME)

C1 N

RN 429689-81-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-chloro-5,6-dihydro-5-methyl- (9CI) (CA INDEX NAME)

RN 429689-82-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-chloro-5,6-dihydro-10-methyl- (9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 4 OF 10 CAPLUS COPYRIGHT 2003 ACS
L4
     2002:389415 CAPLUS
AN
DN
     137:232610
     A convenient synthesis of 5- and 8-nitroquinazoline-2,4-dione
TI
     derivatives
ΑU
     Aziane, D.; Soukri, M.; El Hakmaoui, A.; Lazar, S.; Essassi, E. M.;
     Guillaumet, G.; Akssira, M.
     Laboratoire de Chimie Bioorganique et Analytique, FST-Universite Hassan
CS
     II - Mohammedia, Mohammedia, 20650, Morocco
     Journal of Heterocyclic Chemistry (2002), 39(2), 271-276
SO
     CODEN: JHTCAD; ISSN: 0022-152X
PB
     HeteroCorporation
DТ
     Journal
LA
     English
OS
     CASREACT 137:232610
     3-Nitrophthalic acid was converted selectively to the two regioisomeric
AB
     monoesters, which were subsequently transformed via Curtius
rearrangement
     to the corresponding 5- and 8-nitroguinazoline-2,4-diones, resp. The
     redn. of the nitro group produced 5- and 8-aminoquinazoline-2,4-diones,
     resp., in good yields. The cyclocondensation of 8-amino-3-
     phenylquinazoline-2,4(1H,3H)-dione and 8-amino-3-(4-
     methoxyphenyl)quinazoline-2,4(1H,3H)-dione with CS2 in pyridine afforded
     tricyclic derivs., thioxoimidazo[4,5,1-ij]quinazolinediones, which are
     analogs of the HIV-1 reverse transcriptase inhibitor 4,5,6,7-tetrahydro-
5-
     methylimidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-one (TIBO).
ΙŤ
     459146-65-7P 459146-66-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT
     (Reactant or reagent)
        (prepn. of quinazolinediones by Curtius rearrangement of phthalates)
     459146-65-7 CAPLUS
RN
     4H-Imidazo[4,5,1-ij]quinazoline-4,6(5H)-dione, 1,2-dihydro-5-phenyl-2-
CN
     thioxo- (9CI) (CA INDEX NAME)
```

RN 459146-66-8 CAPLUS

4H-Imidazo[4,5,1-ij]quinazoline-4,6(5H)-dione, 1,2-dihydro-5-(4-CN methoxyphenyl)-2-thioxo- (9CI) (CA INDEX NAME)

THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 25 ALL CITATIONS AVAILABLE IN THE RE FORMAT

App's

```
ANSWER 5 OF 10 CAPLUS COPYRIGHT 2003 ACS
L4
     2001:225212 CAPLUS
AN
DN
     134:266331
     Preparation of 2-phenyl-5,6-dihydro-imidazo[4,5,1-jk][1,4]benzodiazepin-
ΤI
     7(4H)-ones as poly(ADP ribose) polymerase inhibitors.
IN
     Lubisch, Wilfried; Kock, Michael; Hoeger, Thomas; Grandel, Roland;
     Mueller, Reinhold; Schult, Sabine
     BASF A.-G., Germany
PA
SO
     Ger. Offen., 12 pp.
     CODEN: GWXXBX
     Patent
DT
     German
LΑ
FAN.CNT 2
                                           APPLICATION NO.
     PATENT NO.
                      KIND DATE
                                                            DATE
                                           -----
                      ____
                            _____
                            20010329
                                           DE 1999-19946289 19990928
ΡI
     DE 19946289
                       A1
                                           WO 2000-EP9023
                       A2
                            20010405
                                                            20000915
     WO 2001023386
                      A3
                            20020510
     WO 2001023386
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     WO 2001023390
                                          WO 2000-EP9024
                            20010405
                      A2
     WO 2001023390
                       А3
                            20011227
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     BR 2000007174
                            20010904
                                          BR 2000-7174
                                                            20000915
                       Α
                            20020306
                                          EP 2000-974379
                                                            20000915
                       A2
     EP 1183259
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     BR 2000014326
                            20020528
                                           BR 2000-14326
                                                             20000915
                       Α
                            20020717
                                           EP 2000-966022
                                                             20000915
     EP 1222191
                       A2
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL
                                           JP 2001-526538
                            20030318
                                                             20000915
     JP 2003510324
                       Т2
                                           JP 2001-526542
     JP 2003510328
                       Т2
                            20030318
                                                             20000915
                                           NO 2001-2567
                                                             20010525
     NO 2001002567
                       Α
                            20010625
                                           BG 2001-105650
                                                            20010626
                       Α
                            20020228
     BG 105650
     BG 6444
                       Α
                            20020930
                                           BG 2002-6444
                                                            20020226
     BG 106444
                            20020930
                                           BG 2002-106444
                                                            20020226
                       Α
     NO 2002001379
                            20020320
                                           NO 2002-1379
                                                            20020320
                       Α
PRAI DE 1999-19946289
                       Α
                            19990928
     DE 2000-10039610
                       Α
                            20000809
     WO 2000-EP9023
                       W
                            20000915
     WO 2000-EP9024
                       W
                            20000915
```

$$X^1$$
 $X^2$ 
 $X^3$ 
 $X^3$ 
 $X^3$ 

AB Title compds. [I; A = (substituted) C1-3 alkylene; X1 = S, O, NE; X2 = N, (substituted) C; X3 = N, CR2; R2 = H, alkyl, alkylphenyl, Ph; R1 = H, halo, OH, NO2, CF3, cyano, alkyl, alkoxy, etc.; B = (unsatd.) (O-, N-, S-interrupted) (substituted) mono-, bi-, tricyclyl] were prepd. as poly(ADP ribose) polymerase inhibitors (no data). Thus, Me 2-chloro-3-nitrobenzoate was heated with K2CO3 and H2NCH2CH2NH2 in DMF for 3 at 120.degree. to give 9-nitro-1,2,3,4-tetrahydro-5H-1,4-benzodiazepin-5-one, which was hydrogenated using Pd/C in EtOH to give 9-amino-1,2,3,4-tetrahydro-5H-1,4-benzodiazepin-5-one. The latter in MeOH contg. HOAc was treated dropwise with 4-(4-methylpiperazin-1-yl)benzaldehyde in MeOH followed by 1 h stirring at room temp.; Cu(OAc)2, Na2S, and HCl in H2O were added followed by 30 min reflux to give 2-[4-(4-methylpiperazin-1-yl)phenyl]-5,6-dihydro-imidazo[4,5,1-ik][1,4]benzodiazepin-7(4H)-one.

331730-18-8P 331730-20-2P 331730-21-3P 331730-22-4P 331730-23-5P 331730-24-6P 331730-26-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of phenyldihydroimidazobenzodiazepinones as PARP inhibitors)

RN 331730-18-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-methyl-1-piperazinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 331730-20-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[2-(diethylamino)ethoxy]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 331730-21-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

η,

RN 331730-22-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[2-(diethylamino)ethyl]methylamino]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 331730-23-5 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]-, 1,1-dimethylethyl

ester (9CI) (CA INDEX NAME)

RN 331730-24-6 CAPLUS

CN 1H-1,4-Diazepine-1-carboxylic acid, hexahydro-4-[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 331730-26-8 CAPLUS

CN 1H-1,4-Diazepine-1-carboxylic acid, hexahydro-4-[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]-, 1,1-dimethylethyl ester, trihydrochloride (9CI) (CA INDEX NAME)

IT 331730-19-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of phenyldihydroimidazobenzodiazepinones as PARP inhibitors)
331730-19-9 CAPLUS

RN 331730-19-9 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

```
ANSWER 6 OF 10 CAPLUS COPYRIGHT 2003 ACS
L4
     2001:167995 CAPLUS
AN
DN
     134:207833
     Preparation of tricyclic inhibitors of poly(ADP-ribose) polymerases
ΤI
     Webber, Stephen Evan; Skalitzky, Donald James; Tikhe, Jayashree Girish;
IN
     Kumpf, Robert Arnold; Marakovits, Joseph Timothy; Eastman, Walter Brian
     Agouron Pharmaceuticals, Inc., USA; Cancer Research Campaign Technology
PΑ
     Limited
SO
     PCT Int. Appl., 236 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
                      KIND DATE
                                           APPLICATION NO.
                                                           DATE
     PATENT NO.
                      ----
                                           _____
                            -----
     WO 2001016136
                      A2
                            20010308
                                           WO 2000-US23882 20000831
PΙ
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
             CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
             ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
             LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,
             SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW,
             AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                           20020529
                                         EP 2000-961437 20000831
     EP 1208104
                      A2
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL
                                           BR 2000-15051
                                                            20000831
     BR 2000015051
                       Α
                            20020625
     JP 2003513015
                       Т2
                            20030408
                                           JP 2001-519702
                                                            20000831
     US 6548494
                       В1
                            20030415
                                           US 2000-653184
                                                            20000831
     NO 2002000421
                       Α
                            20020425
                                           NO 2002-421
                                                            20020128
                                           BG 2002-106562
     BG 106562
                       Α
                            20030331
                                                            20020329
PRAI US 1999-152142P
                       Ρ
                            19990831
     WO 2000-US23882
                      W
                            20000831
os
     MARPAT 134:207833
GI
                 Ι
AB
     The title compds. [I; X = O, S; Y = N, CR3 (wherein R3 = halo, CN,
```

AB The title compds. [I; X = O, S; Y = N, CR3 (wherein R3 = halo, CN, alkyl, etc.); R1 = H, halo, CN, etc.; R2 = H, alkyl; R4 = H, halo, alkyl; R5-R8 = H, alkyl, alkenyl, aryl, etc.] which are poly(ADP-ribosyl)transferase inhibitors, and are useful in treating cancers and in ameliorating the effects of stroke, head trauma, and neurodegenerative disease, were prepd. E.g., a multi-step synthesis of 1-phenyl-8,9-dihydro-7H-2,7,9a-triaza-benzo[cd]azulen-6-one [I; Y = N; X = O; R1 = Ph; R2, R4-R8 = H] was given. Biol. data for compds. I were presented.

IT 328542-04-7P 328542-20-7P 328542-32-1P 328542-56-9P 328542-58-1P 328542-59-2P

328542-61-6P 328543-05-1P 328543-07-3P 328543-09-5P 328543-29-9P 328543-31-3P 328543-41-5P 328543-50-6P 328544-89-2P 328544-00-9P 328544-08-7P 328544-29-2P 328544-34-9P 328544-48-5P 328544-55-4P 328544-57-6P 328544-61-2P 328544-63-4P 328544-65-6P 328544-71-4P 328544-77-0P 328544-83-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of tricyclic inhibitors of poly(ADP-ribose) polymerases) 328542-04-7 CAPLUS

RN 328542-04-7 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-phenyl(9CI) (CA INDEX NAME)

RN 328542-20-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 328542-32-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(2-chloro-4-pyridinyl)-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328542-56-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 1,2,5,6-tetrahydro-2-thioxo-(9CI) (CA INDEX NAME)

RN 328542-58-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)

RN 328542-59-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-(1,3-dioxan-2-yl)phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328542-61-6 CAPLUS

CN Benzaldehyde, 3-(4,5,6,7-tetrahydro-7-oxoimidazo(4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 328543-05-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(diethoxymethyl)phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328543-07-3 CAPLUS

CN Benzaldehyde, 4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 328543-09-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(dimethylamino)methyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328543-29-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-(1,3-dioxolan-2-yl)phenyl]-9-fluoro-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328543-31-3 CAPLUS

CN Benzaldehyde, 3-(9-fluoro-4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 328543-41-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepine-2-carboxylic acid, 4,5,6,7-tetrahydro-7-oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 328543-50-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(diethoxymethyl)phenyl]-9-fluoro-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328543-84-6 CAPLUS

CN Imidazo $\{4,5,1-jk\}$ [1,4]benzodiazepin-7(4H)-one, 9-fluoro-5,6-dihydro-2-[4-

(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-00-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-thiomorpholinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-08-7 CAPLUS

CN Benzonitrile, 4-[[5-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)-2-pyridinyl]oxy]- (9CI) (CA INDEX NAME)

RN 328544-29-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(2-hydroxyethoxy)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-34-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[2-(1-pyrrolidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)

RN 328544-38-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[2-(tetrahydro-2H-pyran-2-yl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328544-40-7 CAPLUS .

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(2-pyridinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-42-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-48-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(2-piperidinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-55-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(3-pyridinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-57-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-pyridinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-61-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-piperidinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-63-4 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(methylthio)(9CI) (CA INDEX NAME)

RN 328544-65-6 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 328544-71-4 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(3-piperidinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-77-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 328544-83-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(2-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

 IT
 328542-06-9P
 328542-08-1P
 328542-10-5P

 328542-12-7P
 328542-14-9P
 328542-16-1P

 328542-18-3P
 328542-22-9P
 328542-24-1P

 328542-26-3P
 328542-36-5P
 328542-30-9P

 328542-34-3P
 328542-36-5P
 328542-38-7P

 328542-40-1P
 328542-42-3P
 328542-43-4P

 328542-45-6P
 328542-46-7P
 328542-48-9P

 328542-50-3P
 328542-52-5P
 328542-54-7P

 328542-63-8P
 328542-99-0P
 328543-01-7P

 328543-03-9P
 328543-11-9P
 328543-13-1P

 328543-15-3P
 328543-17-5P
 328543-19-7P

```
328543-21-1P 328543-23-3P 328543-25-5P
     328543-27-7P 328543-33-5P 328543-35-7P
     328543-37-9P 328543-39-1P 328543-43-7P
     328543-45-9P 328543-47-1P 328543-49-3P
     328543-52-8P 328543-78-8P 328543-80-2P
     328543-82-4P 328543-86-8P 328543-89-1P
     328543-91-5P 328543-92-6P 328543-94-8P
     328543-96-0P 328543-98-2P 328544-02-1P
     328544-04-3P 328544-06-5P 328544-10-1P
     328544-12-3P 328544-14-5P 328544-16-7P
     328544-18-9P 328544-20-3P 328544-22-5P
     328544-23-6P 328544-25-8P 328544-27-0P
     328544-31-6P 328544-33-8P 328544-36-1P
     328544-44-1P 328544-46-3P 328544-49-6P
     328544-51-0P 328544-53-2P 328544-59-8P
     328544-67-8P 328544-69-0P 328544-73-6P
     328544-75-8P 328544-79-2P 328544-81-6P
     328544-85-0P 328544-87-2P 328544-89-4P
     328544-91-8P 328545-24-0P 328545-25-1P
     328545-28-4P 328545-30-8P 328545-31-9P
     328545-33-1P 328545-34-2P 328545-37-5P
     328545-40-0P 328545-43-3P 328545-46-6P
     328545-48-8P 328545-51-3P 328545-54-6P
     328545-57-9P 328545-60-4P 328545-63-7P
     328545-66-0P 328545-69-3P 328545-72-8P
     328545-75-1P 328545-78-4P 328545-81-9P
     328545-84-2P 328545-86-4P 328545-89-7P
     328545-91-1P 328545-94-4P 328545-97-7P
     328545-99-9P 328546-02-7P 328546-05-0P
     328546-07-2P 328546-09-4P 328546-13-0P
     328546-15-2P 328546-17-4P 328546-18-5P
     328546-20-9P 328546-21-0P 328546-22-1P
     328546-23-2P 328546-25-4P 328546-26-5P
     328546-27-6P 328546-28-7P 328546-29-8P
     328546-31-2P 328546-32-3P 328546-33-4P
     328546-34-5P 328546-36-7P 328546-38-9P
     328546-39-0P 328546-40-3P 328546-41-4P
     328546-42-5P 328546-43-6P 328546-44-7P
     328546-45-8P 328546-46-9P 328546-47-0P
     328546-48-1P 328546-49-2P 328546-50-5P
     328546-51-6P 328546-52-7P 328546-53-8P
     328546-54-9P 328546-55-0P 328546-56-1P
     328546-57-2P 328546-58-3P 328546-59-4P
     328546-60-7P 328546-61-8P 328546-62-9P
     RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic
use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of tricyclic inhibitors of poly(ADP-ribose) polymerases)
     328542-06-9 CAPLUS
     Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-fluorophenyl)-5,6-
     dihydro- (9CI) (CA INDEX NAME)
```

RN

CN

RN 328542-08-1 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(4-pyridinyl)(9CI) (CA INDEX NAME)

RN 328542-10-5 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(3,4-difluorophenyl)5,6dihydro- (9CI) (CA INDEX NAME)

RN 328542-12-7 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(2-chlorophenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328542-14-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(3-phenoxyphenyl)- (9CI) (CA INDEX NAME)

328542-16-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(3-pyridinyl)-

(9CI) (CA INDEX NAME)

RN

RN 328542-18-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-thienyl)-

(9CI) (CA INDEX NAME)

RN 328542-22-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328542-24-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 328542-26-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-pyridinyl)-

(9CI) (CA INDEX NAME)

RN 328542-28-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(5-isoxazolyl)- (9CI) (CA INDEX NAME)

RN 328542-30-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-chlorophenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328542-34-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(3-pyridinyloxy)phenyl]- (9CI) (CA INDEX NAME)

RN 328542-36-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(4-pyridinyloxy)phenyl]- (9CI) (CA INDEX NAME)

RN 328542-38-7 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-fluoro-2-(4-fluorophenyl) 5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328542-40-1 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-phenylethyl)- (9CI) (CA INDEX NAME)

RN 328542-42-3 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(2-furanyl)-5,6-dihydro(9CI) (CA INDEX NAME)

RN 328542-43-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 328542-45-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(1,1-dimethylethyl)-5,6-

dihydro- (9CI) (CA INDEX NAME)

RN 328542-46-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-methylpropyl)- (9CI) (CA INDEX NAME)

RN 328542-48-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-cyclohexyl-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328542-50-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepine-7(4H)-thione, 5,6-dihydro-2-phenyl-(9CI) (CA INDEX NAME)

RN 328542-52-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepine-2,7(1H,4H)-dione, 5,6-dihydro-(9CI)

(CA INDEX NAME)

(1 -

RN 328542-54-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-6-methyl-2-

naphthalenyl) - (9CI) (CA INDEX NAME)

RN 328542-63-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-[(dimethylamino)methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328542-99-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepine-2,7(1H,4H)-dione, 5,6-dihydro-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

RN 328543-01-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-chlorophenyl)-5,6-dihydro-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

RN 328543-03-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-(1,3-dioxolan-2-yl)phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-11-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-[(methylamino)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328543-13-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(1-pyrrolidinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328543-15-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-[3-(trifluoromethyl)phenoxy]phenyl]- (9CI) (CA INDEX NAME)

RN 328543-17-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-(4-chlorophenoxy)phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328543-19-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-(3,4-dichlorophenoxy)phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328543-21-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(4-methoxyphenoxy)phenyl]- (9CI) (CA INDEX NAME)

RN 328543-23-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-(3,5-dichlorophenoxy)phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328543-25-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(3-benzoylphenyl)-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328543-27-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(phenylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328543-33-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-[(dimethylamino)methyl]phenyl]-9-fluoro-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-35-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[2-(dimethylamino)-4-pyridinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

[3-

RN 328543-37-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-fluoro-5,6-dihydro-2-

[(methylamino)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328543-39-1 CAPLUS

CN Benzonitrile, 3-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 328543-43-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(methylamino)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328543-45-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-morpholinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328543-47-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(2-methoxyethyl)amino]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328543-49-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

RN 328543-52-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1H-imidazol-

2-yl)- (9CI) (CA INDEX NAME)

RN 328543-78-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(2-thiazolyl)-

(9CI) (CA INDEX NAME)

RN 328543-80-2 CAPLUS CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1H-pyrrol-2-yl)- (9CI) (CA INDEX NAME)

RN 328543-82-4 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[5-(4-chlorophenyl)-2-furanyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-86-8 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-fluoro-5,6-dihydro-2[4[(methylamino)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328543-91-5 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[(2-ethoxyethyl)amino]methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-92-6 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4[(cyclopropylamino)methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328543-94-8 CAPLUS

CN Acetonitrile, [[[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

RN 328543-96-0 CAPLUS

CN Imidazo $\{4,5,1-jk\}$ [1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2- $[4-\{[2,2,2-]$ 

trifluoroethyl)amino]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328543-98-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(2-propynylamino)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$HC = C - CH2 - NH - CH2$$

RN 328544-02-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[2-(4-methylphenyl)-4-thiazolyl]- (9CI) (CA INDEX NAME)

RN 328544-04-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[3-(4-methylphenyl)-2,1-benzisoxazol-5-yl]- (9CI) (CA INDEX NAME)

RN 328544-06-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[6-[(4-chlorophenyl)thio]-

3-pyridinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328544-10-1 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepine-2-carboxamide, 4,5,6,7-tetrahydro7oxo-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 328544-12-3 CAPLUS
CN Propanenitrile, 3-[[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

RN 328544-14-5 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 328544-16-7 CAPLUS

CN Morpholine, 4-[(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)

RN 328544-18-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[1,6-dihydro-6-oxo-1-(phenylmethyl)-3-pyridinyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328544-20-3 CAPLUS

CN Piperazine, 1-methyl-4-[(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)

RN 328544-22-5 CAPLUS

CN Benzamide, 4-[[5-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)-2-pyridinyl]oxy]- (9CI) (CA INDEX NAME)

RN 328544-23-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-tricyclo[3.3.1.13,7]dec-1-yl- (9CI) (CA INDEX NAME)

RN 328544-25-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(6-chloro-3-pyridinyl)-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328544-27-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1H-imidazol-1-yl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-31-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[3-(dimethylamino)propoxy]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328544-33-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(1-oxido-

4-thiomorpholinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328544-36-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[2-(dimethylamino)ethoxy]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328544-44-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[2-(1-pyrrolidinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328544-46-3 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[2-(dimethylamino)ethyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

Me2N—CH2—CH2

RN 328544-49-6 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4[(dimethyloxidoamino)methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328544-51-0 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-methyl2-piperidinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-53-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(2-methyl-

2H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-59-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-67-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(methylsulfonyl)- (9CI) (CA INDEX NAME)

RN 328544-69-0 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-methyl-4-piperidinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-73-6 CAPLUS
CN 1-Piperidinecarboxylic acid, 3-[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 328544-75-8 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-methyl-3-piperidinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-79-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-amino-5,6-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 328544-81-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1H-imidazol-4-yl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-85-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-methyl-

2-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328544-87-2 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[1-(cyclopropylmethyl)2-piperidinyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328544-89-4 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[1-(1-methylethyl)-2-piperidinyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328544-91-8 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1H-imidazol-2-yl)phenyl]- (9CI) (CA INDEX NAME)

RN 328545-24-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-lH-pyrrol-1-yl)methyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328545-25-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-fluoro-5,6-dihydro-2-

[4-[(3-hydroxy-1-pyrrolidinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328545-28-4 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(2R)-2-(hydroxymethyl)-1-pyrrolidinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328545-30-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(3-hydroxy-1-pyrrolidinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328545-31-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[3-(hydroxymethyl)-1-piperidinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328545-33-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-{4-[[(2,3-dihydroxypropyl)methylamino]methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328545-34-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-1H-pyrrol-1-yl)methyl]phenyl]-9-fluoro-5,6-dihydro-(9CI) (CA INDEX NAME)

CM 2

CRN 76-05-1

CMF C2 H F3 O2

RN 328545-40-0 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4[[methyl(2phenylethyl)amino]methyl]phenyl]-, trifluoroacetate (5:3) (9CI) (CA · INDEX
NAME)

CM 1

CRN 328545-39-7 CMF C26 H26 N4 O

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-43-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[butyl(2-hydroxyethyl)amino]methyl]phenyl]-5,6-dihydro-, trifluoroacetate (5:3) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-42-2 CMF C23 H28 N4 O2

CM 2

CRN 76-05-1

RN 328545-46-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(2S)-2-

(hydroxymethyl)-1-pyrrolidinyl]methyl]phenyl]-, mono(trifluoroacetate)
(salt) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-45-5 CMF C22 H24 N4 O2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-48-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(3,6-dihydro-1(2H)-pyridinyl)methyl]phenyl]-5,6-dihydro-, trifluoroacetate (20:17) (9CI)

(CA INDEX NAME)

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-51-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(2-phenylethyl)amino]methyl]phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX

NAME)

CM 1

CRN 328545-50-2 CMF C25 H24 N4 O

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-54-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[[2-(3-methoxyphenyl)ethyl]amino]methyl]phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-53-5 CMF C26 H26 N4 O2

PAGE 1-A

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-57-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[[2-(4-fluorophenyl)ethyl]amino]methyl]phenyl]-5,6-dihydro-, trifluoroacetate (5:8) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-56-8 CMF C25 H23 F N4 O

PAGE 1-A

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-60-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[[2-(4-methoxyphenyl)ethyl]amino]methyl]phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-59-1 CMF C26 H26 N4 O2

PAGE 1-A

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-63-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[methyl(2-

methylpropyl)amino]methyl]phenyl]-, mono(trifluoroacetate) (9CI) (CA
INDEX NAME)

CM 1

CRN 328545-62-6 CMF C22 H26 N4 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-66-0 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4[(cyclobutylamino)methyl]phenyl]-5,6-dihydro-, mono(trifluoroacetate)
(9CI) (CA INDEX NAME)

CM 1

CRN 328545-65-9 CMF C21 H22 N4 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-69-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(2-thienylmethyl)amino]methyl]phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-68-2

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-72-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(dipropylamino)methyl]phenyl]-5,6-dihydro-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-71-7 CMF C23 H28 N4 O

RN 328545-75-1 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[(1,3-benzodioxol-5-ylmethyl)amino]methyl]phenyl]-5,6-dihydro-, trifluoroacetate (4:9) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-74-0 CMF C25 H22 N4 O3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-78-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[(2,3-dihydro-1H-inden-1-yl)amino]methyl]phenyl]-5,6-dihydro-, trifluoroacetate (10:19) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-77-3 CMF C26 H24 N4 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-81-9 CAPLUS

CN .beta.-Alanine, N-(2-furanylmethyl)-N-[[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]methyl]-, ethyl ester,

trifluoroacetate (4:7) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-80-8 CMF C27 H28 N4 O4

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-84-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[[2-(1-methyl-2-pyrrolidinyl)ethyl]amino]methyl]phenyl]-, trifluoroacetate (4:13)

(9CI) (CA INDEX NAME)

CM 1

CRN 328545-83-1 CMF C24 H29 N5 O

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-86-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[[(5-methyl-2-furanyl)methyl]amino]methyl]phenyl]-, trifluoroacetate (4:5) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-85-3 CMF C23 H22 N4 O2

PAGE 2-A

1/2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-89-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(phenylmethyl)amino]methyl]phenyl]-, trifluoroacetate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-88-6 CMF C24 H22 N4 O

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-91-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[(2,3-dihydro-1H-inden-2-yl)amino]methyl]phenyl]-5,6-dihydro-, bis(trifluoroacetate) (9CI)

(CA INDEX NAME)

CM 1

CRN 328545-90-0 CMF C26 H24 N4 O

RN 328545-94-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(3,4-dihydro-2(1H)-isoquinolinyl)methyl]phenyl]-5,6-dihydro-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-93-3 CMF C26 H24 N4 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-97-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[methyl(phenylmethyl)amino]methyl]phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME) CM :

CRN 328545-96-6 CMF C25 H24 N4 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328545-99-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(2-phenylpropyl)amino]methyl]phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX

NAME)

CM 1

CRN 328545-98-8 CMF C26 H26 N4 O

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-02-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[(3-phenylpropyl)amino]methyl]phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX

NAME)

CM 1

CRN 328546-01-6 CMF C26 H26 N4 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-05-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[methy][2-

(2-pyridinyl)ethyl]amino]methyl]phenyl]-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-04-9 CMF C25 H25 N5 O

PAGE 1-A

PAGE 2-A

CM 2

CRN 76-05-1

RN 328546-07-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[ethyl[2-(2-pyridinyl)ethyl]amino]methyl]phenyl]-5,6-dihydro-,

tris(trifluoroacetate)

(9CI) (CA INDEX NAME)

CM 1

CRN 328546-06-1 CMF C26 H27 N5 O

PAGE 1-A

RN 328546-09-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[[2-(2-pyridinyl)ethyl]amino]methyl]phenyl]-, trifluoroacetate (4:9) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-08-3 CMF C24 H23 N5 O

PAGE 1-A

RN 328546-13-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[methyl[2-

(4-pyridinyl)ethyl]amino]methyl]phenyl]-, trifluoroacetate (2:7) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-12-9 CMF C25 H25 N5 O

PAGE 1-A

RN 328546-15-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[[2-(4-pyridinyl)ethyl]amino]methyl]phenyl]-, trifluoroacetate (4:13) (9CI)

(CA

INDEX NAME)

CM 1

CRN 328546-14-1 CMF C24 H23 N5 O

PAGE 1-A

RN 328546-17-4 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[[[2-(1H-indol-2-yl)ethyl]methylamino]methyl]phenyl]-, trifluoroacetate (2:5)
(9CI)
(CA INDEX NAME)

CM 1

CRN 328546-16-3 CMF C28 H27 N5 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-18-5 CAPLUS CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(azidomethyl)phenyl]-

5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328546-20-9 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(aminomethyl)phenyl]5,6-dihydro-, trifluoroacetate (4:7) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-19-6 CMF C17 H16 N4 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-21-0 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-pyrrolidinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328546-22-1 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-fluoro-5,6-dihydro-2[4(1-pyrrolidinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328546-25-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1H-imidazol-1-ylmethyl)phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-24-3 CMF C20 H17 N5 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-26-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dimethyl-1-pyrrolidinyl)methyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328546-27-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(1,3,3-trimethyl-6-azabicyclo[3.2.1]oct-6-yl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328546-28-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[[(2S,5S)-2,5-bis(methoxymethyl)-1-pyrrolidinyl]methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

RN 328546-31-2 CAPLUS
CN D-Proline, 1-[[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]methyl]-, 1,1-dimethylethyl ester, trifluoroacetate (4:3) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-30-1 CMF C26 H30 N4 O3

Absolute stereochemistry.

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-32-3 CAPLUS

CN Carbamic acid, [1-[[4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)phenyl]methyl]-3-pyrrolidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 328546-33-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1H-pyrrol-

1-ylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328546-34-5 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4[(dimethylamino)methyl]phenyl]-5,6-dihydro-5-methyl-, (5S)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 328546-36-7 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-methyl-2[4[(methylamino)methyl]phenyl]-, (5S)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-35-6 CMF C19 H20 N4 O

Absolute stereochemistry.

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-38-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-1H-pyrrol-1-yl)methyl]phenyl]-5,6-dihydro-5-methyl-, (5S)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 328546-37-8 CMF C22 H22 N4 O

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 328546-39-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-1H-pyrrol-1-yl)methyl]phenyl]-5,6-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

RN 328546-40-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-1H-pyrrol-1-yl)methyl]phenyl]-5,6-dihydro-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 328545-24-0 CMF C21 H20 N4 O

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 328546-41-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-1H-pyrrol-1-yl)methyl]phenyl]-5,6-dihydro-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 328545-24-0 CMF C21 H20 N4 O

CM 2

CRN 75-75-2 CMF C H4 O3 S

RN 328546-42-5 CAPLUS

CN Benzonitrile, 4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 328546-43-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-hydroxy-

3-methylbutyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328546-44-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[1-(2,5-dihydro-1H-pyrrol-1-yl)-3-methylbutyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328546-45-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[3-methy]-

1-(1-pyrrolidinyl)butyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328546-46-9 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[1-(dimethylamino)-3methylbutyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328546-47-0 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-1H-pyrrol-1-yl)methyl]phenyl]-9-fluoro-5,6-dihydro-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 328545-34-2

CMF C21 H19 F N4 O

CM 2

CRN 75-75-2 CMF C H4 O3 S

RN 328546-48-1 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-methyl-2[4(1-pyrrolidinylmethyl)phenyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-49-2 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-methyl-2[4(1H-pyrrol-1-ylmethyl)phenyl]-, (5S)- (9CI) (CA INDEX NAME)

RN 328546-50-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-chlorophenyl)-5,6-dihydro-5-methyl-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-51-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-chlorophenyl)-5,6-dihydro-5-methyl-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-52-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-chlorophenyl)-5,6-dihydro-5-(hydroxymethyl)-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-54-9 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5(hydroxymethyl)-2-[4-[[methyl(2-phenylethyl)amino]methyl]phenyl]-, (5R)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-56-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-(hydroxymethyl)-2-[4-(1-pyrrolidinylmethyl)phenyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328546-57-2 CAPLUS

CN Benzeneacetonitrile, 4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

RN 328546-58-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dihydro-2,5-dimethyl-1H-pyrrol-1-yl)methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328546-59-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(2,5-dimethyl-1H-pyrrol-1-yl)methyl]phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328546-60-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[1-(dimethylamino)ethyl]phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

RN 328546-61-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[1-(1-pyrrolidinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 328546-62-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[2-phenyl-

1-(1-pyrrolidinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

## IT 328546-76-5P 328546-77-6P 328547-34-8P

RL: BYP (Byproduct); PREP (Preparation)

(prepn. of tricyclic inhibitors of poly(ADP-ribose) polymerases)

RN 328546-76-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[3-

(dimethoxymethyl)phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328547-34-8 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[(1E)-2-phenylethenyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

328546-95-8 CAPLUS

CN Benzaldehyde, 4-(9-fluoro-4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

328546-96-9 CAPLUS RN

Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[2-CN [(methylsulfonyl)oxy]ethoxy]phenyl]- (9CI) (CA INDEX NAME)

RN 328547-10-0 CAPLUS

Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(chloromethyl)phenyl]-

5,6-dihydro- (9CI) (CA INDEX NAME)

328547-13-3 CAPLUS RN

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4(chloromethyl)phenyl] 9-fluoro-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328547-15-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-{4-(hydroxymethyl)phenyl]-5-methyl-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328547-16-6 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(chloromethyl)phenyl]5,6-dihydro-5-methyl-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328547-17-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(2-chloro-3-methylbutyl)phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328547-21-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-chlorophenyl)-5,6-dihydro-5-[(phenylmethoxy)methyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328547-23-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(hydroxymethyl)phenyl]-5-[(phenylmethoxy)methyl]-, (5R)- (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 328547-24-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(chloromethyl)phenyl]-

5,6-dihydro-5-[(phenylmethoxy)methyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328547-25-7 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(chloromethyl)phenyl]5,6-dihydro-5-(hydroxymethyl)-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 328547-26-8 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328547-28-0 CAPLUS
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(1-chloroethyl)phenyl]5,6-dihydro- (9CI) (CA INDEX NAME)

RN 328547-30-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-hydroxy-

2-phenylethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328547-32-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(1-chloro-2-phenylethyl)phenyl]-5,6-dihydro-(9CI) (CA INDEX NAME)

## IT 328546-89-0P 328547-22-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of tricyclic inhibitors of poly(ADP-ribose) polymerases)

RN 328546-89-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328547-22-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5-(bromomethyl)-2-(4-chlorophenyl)-5,6-dihydro-, (5R)- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2003 ACS

AN 1995:380741 CAPLUS

DN 122:290829

TI Synthesis and Anti-HIV-1 Activity of 4,5,6,7-Tetrahydro-5-methylimidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-one (TIBO) Derivatives.

AU Breslin, Henry J.; Kukla, Michael J.; Ludovici, Donald W.; Mohrbacher, Richard; Ho, Winston; Miranda, Milton; Rodgers, James D.; Hitchens, T. Kevin; Leo, Gregory; et al.

CS Janssen Research Foundation, Spring House, PA, 19477, USA

SO Journal of Medicinal Chemistry (1995), 38(5), 771-93 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

GI

4,5,6,7-Tetrahydro-5-methylimidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-AB ones (TIBO) (I, R = H, 5-Et, 7-Ph, etc.; X = S, O; Y = 8-C1, 9-C1; Z =H, 3,3-dimethylallyl, Pr, etc.) have been shown to significantly inhibit HIV-1 replication in vitro by interfering with the virus's reverse transcriptase enzyme. We describe our synthetic endeavors around 4, 5, and 7 mono- and disubstitutions of I and discuss HIV-1 inhibitory structure-activity relationships. On the basis of inhibition of HIV-1 replication in MT-4 cells, we found that 5-mono-Me-substituted analogs and 7-mono-Me-substituted analogs of I were comparable as being consistently the most active compds. Although generally less active, the 4,5,7-unsubstituted, 4-mono-substituted, cis- and trans-5,7-di-Mesubstituted, and cis-4,5-di-Me-substituted analogs of I also exhibited significant activity. The remaining trans-4,5-di-Me-substituted, cisand trans-4,7-di-Me-substituted, and all 4,5-, 5,6-, 6,7-, and 7,8-fused disubstituted analogs of I possessed no noticeable desired activity.

IT 162930-41-8P 162930-45-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (synthesis and anti-HIV-1 activity of imidazobenzodiazepinones)

RN 162930-41-8 CAPLUS

CN Benz[b]imidazo[4,5,1-jk][1,4]benzodiazepin-6(7H)-one, 1,2-dihydro-1-thioxo-(9CI) (CA INDEX NAME)

RN 162930-45-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepine-2,7(1H,4H)-dione, 5,6-dihydro-5-methyl-6-propyl- (9CI) (CA INDEX NAME)

-

.

L4 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2003 ACS

AN 1991:632195 CAPLUS

DN 115:232195

TI Synthesis and anti-HIV-1 activity of 4,5,6,7-tetrahydro-5-methylimidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-one (TIBO) derivatives.

AU Kukla, Michael J.; Breslin, Henry J.; Diamond, Craig J.; Grous, Philip P.; Ho, Chih Y.; Miranda, Milton; Rodgers, James D.; Sherrill, Ronald G.; De Clercq, Erik; et al.

CS Janssen Res. Found., Spring House, PA, 19477, USA

SO Journal of Medicinal Chemistry (1991), 34(11), 3187-97 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

GI

AB Potential anti-HIV-1 imidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-one I (R = R1 = H, X = O) analogs with variations of the five-membered urea ring were prepd. Although many different rings were synthesized to replace the cyclic urea of I, most were found to be inactive in inhibiting the replication of the HIV-1 virus in MT-4 cells. The exceptions were replacement of the urea oxygen with sulfur or selenium to give the corresponding thio- or selenoureas. These were found to be more active than the oxygen counterparts. A small series of analogs were synthesized and tested which allowed direct comparison of urea and thiourea derivs. Without exception, the latter were always more active than the former. The most active compd. (S)(+)-I (R = CH2C:CEt2, R1 = C1, X = S) was found to inhibit the HIV-1 virus with an IC50 of 0.012 .mu.M which is comparable to that of AZT.

IT 136722-95-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and redn. of)

RN 136722-95-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-methyl-(9CI) (CA INDEX NAME)

L4 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2003 ACS

AN 1978:507034 CAPLUS

DN 89:107034

TI Fragmentation in mass spectrometry of imidazobenzodiazepines

AU Geneste, Patrick; Kamenka, Jean Marc; Vidal, Yves

CS Lab. Chim. Org. Phys. Appl., Ec. Natl. Super. Chim., Montpellier, Fr.

SO Organic Mass Spectrometry (1978), 13(3), 141-53 CODEN: ORMSBG; ISSN: 0030-493X

DT Journal

LA French

AB Mass spectra are reported for 7 imidazo[1,5,4-ef]-1,5- and 11 imidazo[4,5,1-jk]-1,4-benzodiazepines. Differences in fragmentation patterns enabled isomeric structures to be identified.

IT 66596-57-4 66596-59-6 66596-60-9

66596-64-3 66596-69-8

RL: PRP (Properties) (mass spectrum of)

RN 66596-57-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-chloro-5,6-dihydro-2-methyl- (9CI) (CA INDEX NAME)

RN 66596-59-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-chloro-5,6-dihydro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 66596-60-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-9-nitro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 66596-64-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-methyl-(9CI)(CA INDEX NAME)

RN 66596-69-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-methyl-9-nitro-(9CI) (CA INDEX NAME)

L4 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2003 ACS

AN 1978:182987 CAPLUS

DN 88:182987

TI Studies on the imidazo[4,5,1-jk][1,4]benzodiazepine and imidazo[1,5,4-ef][1,5]benzodiazepine series

AU Geneste, P.; Kamenka, J. M.; Vidal, Y.; Fauquet, J. P.; Morel, E.; Muller, P.; Warolin, C.

CS Lab. Chim. Org. Phys. Appl., Ec. Natl. Super. Chim., Montpellier, Fr.

SO European Journal of Medicinal Chemistry (1978), 13(1), 53-9 CODEN: EJMCA5; ISSN: 0223-5234

DT Journal

LA French

GΙ

24 1

AB Of the 7 title compds. (I and II, R = Me or PhCH2; X = O; Y = H, Cl, or NO2) prepd., none showed tranquilizing activity in pentetrazole-induced convulsions or mouse motor activity. The prepn. of I and II from imidazoquinolinones (III) is also described.

IT 66596-64-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)

(prepn. and reaction with triethyloxonium fluoroborate)

RN 66596-64-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-methyl-(9CI)(CA INDEX NAME)

IT 66596-57-4P 66596-59-6P 66596-60-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and tranquilizing activity of)

RN 66596-57-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-chloro-5,6-dihydro-2-methyl- (9CI) (CA INDEX NAME)

3~ 1 1 m

RN 66596-59-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 9-chloro-5,6-dihydro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 66596-60-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-9-nitro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)

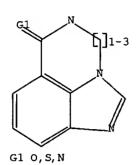
IT 66596-69-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 66596-69-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-methyl-9-nitro-(9CI) (CA INDEX NAME)

=> d l1; d his; log y L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

(FILE 'HOME' ENTERED AT 18:24:31 ON 28 MAY 2003)

FILE 'REGISTRY' ENTERED AT 18:24:38 ON 28 MAY 2003

L1 STRUCTURE UPLOADED

L2 24 S L1

L3 461 S L1 FUL

FILE 'CAPLUS' ENTERED AT 18:25:38 ON 28 MAY 2003

L4 10 S L3

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	46.61	195.37
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-6.51	-6.51

STN INTERNATIONAL LOGOFF AT 18:27:10 ON 28 MAY 2003